3D QSAR WITH MOLECULAR INTERACTION FIELDS BASED ON CONCEPTUAL DFT LOCAL PROPERTIES

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ADME-Tox properties are very important in pharmaceutical research, determining the fate of many molecules in the drug design sequence. Knowledge of ADME-Tox properties in the earliest stages of drug design is therefore highly desirable. The aim of this investigation is to construct low throughput in silico models in which ADME-Tox properties of single compounds are predicted with high accuracy based on Quantum Chemical information[1].

The possible role of quantum chemical information in chemoinformatics is discussed, with a closer look to the advantages, disadvantages and capabilities of quantum chemical descriptors in QSAR environments. The use of quantum chemical fields is investigated by a case study.

[1]M. Karelson Quantum chemical descriptors in QSAR, in: *Computational Medicinal Chemistry for Drug Discoveryi* (Bultinck P, De Winter H, Langenaeker W, Tollenaere JP, eds.) Dekker Inc., NY, pp. 641-667 (2004)